Ground-state energy estimation of molecular systems on physical quantum computers

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Estimating the ground-state energy of quantum systems, such as molecules, is arguably one of the most promising applications of quantum computation. In principle, on near-term quantum computers the problem can be solved by the Variational Quantum Eigensolver (VQE) [1]. In practice, however, chemical applications require generating and measuring entangled trial-states with a high level of accuracy to obtain milli-Hartree precision in the energy estimates, which is made difficult by the presence of noise on present day devices. We have shown that, through quantum computation of the Hamiltonian moments, $\langle \mathcal{H}^n \rangle$, the Quantum Computed Moments (QCM) [2] method, based on Lanczos expansion theory [3, 4], is able to introduce electronic correlations, and hence improve the accuracy, for relatively simple and/or noise limited trial states. For hydrogen atom chains (H_2 to H_6) the QCM method combined with purification techniques was able to estimate the ground state energy with a precision of 0.1 - 10 milli-Hartree on IBM Quantum devices [5]. To move beyond these test models and into the realm of quantum advantage requires scaling to larger systems and presents an array of challenges. Beginning from the test examples we will discuss the challenges that must be overcome to scale the QCM method to the estimation of the ground state energy of H_2O as a starting benchmark. These challenges include: the design of trial circuits to generate sufficient entanglement while minimising noise, the grouping and measurement of large numbers of observables, and the implementation of error mitigation techniques that scale efficiently with both system size and trial state complexity. These problems apply not only to the QCM method but to the VQE in general and so must be overcome if near-term quantum devices are to provide an advantage for quantum chemistry.

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